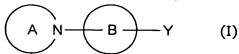
## **CLAIMS**

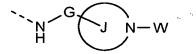
1. A compound represented by formula (I):



wherein ring A represents a nitrogen-containing heterocyclic group which may have a substituent(s); ring B represents a homocyclic group which may have a substituent(s) or a heterocyclic group which may have a substituent(s); and Y represents a hydrocarbon group which may have a substituent(s), a heterocyclic group which may have a substituent(s), an amino group which may be protected, a hydroxyl group which may be protected or a mercapto group which may be protected,

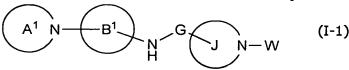
a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof.

- 2. The compound according to claim 1, wherein ring A is a 5- to 10-membered nitrogen-containing heterocyclic group which may have a substituent(s).
- 3. The compound according to claim 1, wherein ring B is a nitrogen-containing heterocyclic group which may have a substituent(s).
  - 4. The compound according to claim 1, wherein Y is



wherein G represents a bond or a spacer containing 1 to 3 atoms as a main chain; ring J represents a 4- to 7-membered nitrogen-containing heterocyclic group which may have a substituent(s); and W represents hydrogen, a hydrocarbon group which may have a substituent(s) or a heterocyclic group which may have a substituent(s).

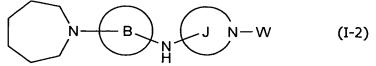
5. The compound according to claim 1, which is represented by formula (I-1):



wherein ring A<sup>1</sup> represents a 5- to 10-membered nitrogen-containing saturated heterocyclic group which may have a substituent(s), or a 5- to 10-membered nitrogen-containing heterocyclic group which has one double bond and which may have a substituent(s); ring B<sup>1</sup> represents a 6- to 11-membered nitrogen-containing monocyclic or

bicyclic heterocyclic group which may have a substituent(s); and other symbols have the same meanings as those described in claim 4.

6. The compound according to claim 1, which is represented by formula (I-2):



wherein all symbols have the same meanings as those described in claim 1 or 4.

7. A compound represented by formula (I-A):

wherein ring A<sup>A</sup> represents a 4- to 15-membered monocyclic, bicyclic or tricyclic heterocyclic group which is saturated or has one double bond and which contains at least one nitrogen atom and may further contain 1 to 3 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom;

ring B<sup>A</sup> represents B<sup>A1</sup> or B<sup>A2</sup>; B<sup>A1</sup> represents:

$$\mathbb{R}^4\mathbb{N}$$
 or

R<sup>4</sup> represents (i) hydrogen, (ii) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl which may be substituted with 1 to 5 of R<sup>10</sup>, (iii) a C3-8 carbocyclic group which may be substituted with 1 to 5 of R<sup>3</sup>, (iv) a 5- to 15-membered heterocyclic group which contains 1 or 2 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom and which may be substituted with 1 to 5 of R<sup>3</sup>, (v) COR<sup>5</sup> wherein R<sup>5</sup> represents C1-15 alkyl, C2-15 alkenyl, C2-15 alkynyl or phenyl, or (vi) COOR<sup>6</sup> wherein R<sup>6</sup> represents C1-15 alkyl, C2-15 alkenyl, C2-15 alkynyl or phenyl; the upward arrow represents a binding position to ring A<sup>A</sup>; and the right-downward arrow represents a binding position to the nitrogen atom bound to L;

L represents (1) a bond, (2) C1-8 alkylene, C2-8 alkenylene or C2-8 alkynylene, wherein the alkylene, alkenylene and alkynylene each may be substituted with 1 to 5 of R<sup>10</sup>, or (3) a C3-8 carbocyclic group which may be substituted with R<sup>3</sup>;

Q represents (1) NR<sup>1</sup>R<sup>2</sup> wherein R<sup>1</sup> and R<sup>2</sup> each independently represents (i) hydrogen, (ii) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl which may be substituted with 1 to 5 of R<sup>10</sup>, (iii) a C3-8 carbocyclic group which may be substituted with 1 to 5 of R<sup>3</sup>, or (iv) a 5- to 15-membered heterocyclic group which contains 1 or 2 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom and which may be substituted 1 to 5 of R<sup>3</sup>, or (2) ring C;

ring C represents a 4- to 15-membered heterocyclic group which contains at least one nitrogen atom and may further contain 1 or 2 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom and which may be substituted with 1 to 5 of R<sup>3</sup>:

plural  $R^3$ 's each independently represents (1) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl, wherein the alkyl, alkenyl and alkynyl may be substituted with 1 to 5 of  $R^{10}$ , (2) oxo, or (3) $R^{10}$ ;

plural R<sup>10</sup>'s each independently represents (1) OR<sup>11</sup>, (2) OCOR<sup>12</sup>, (3) OCOOR<sup>13</sup>, (4) NR<sup>14</sup>R<sup>15</sup>, (5) NR<sup>16</sup>COR<sup>12</sup>, (6) NR<sup>16</sup>CONR<sup>14</sup>R<sup>15</sup>, (7) NR<sup>16</sup>COOR<sup>13</sup>, (8) COOR<sup>13</sup>, (9) COR<sup>12</sup>, (10) CONR<sup>14</sup>R<sup>15</sup>, (11) SO<sub>2</sub>R<sup>12</sup>, (12) SOR<sup>22</sup>, (13) SO<sub>2</sub>NR<sup>24</sup>R<sup>25</sup>, (14) NR<sup>16</sup>SO<sub>2</sub>R<sup>12</sup>, (15) B(OH)<sub>2</sub>, (16) SR<sup>11</sup>, (17) halogen, (18) nitro, (19) cyano, or (20) ring D:

R<sup>11</sup> represents (i) hydrogen, (ii) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl, wherein the alkyl, alkenyl and alkynyl may be substituted with 1 to 5 of halogen, NR<sup>14</sup>R<sup>15</sup>, OR<sup>21</sup>, SR<sup>21</sup>, COOR<sup>13</sup>, or ring D, or (iii) ring D;

R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup> and R<sup>16</sup> each independently represents (i) hydrogen, (ii) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl which may be substituted with ring D, or (iii) ring D;

ring D represents a C3-15 monocyclic, bicyclic or tricyclic carbocyclic group, or a 5- to 15-membered monocyclic, bicyclic or tricyclic heterocyclic group which contains 1 to 4 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom; and

ring D may be substituted with 1 to 5 of the groups selected from the following (1) to (22):

(1) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl, wherein the alkyl, alkenyl or alkynyl may be substituted with 1 to 5 of  $OR^{21}$ ,  $OCOR^{22}$ ,  $OCOOR^{23}$ ,  $NR^{24}R^{25}$ ,  $NR^{26}COR^{22}$ ,  $NR^{26}COR^{24}R^{25}$ ,  $NR^{26}COR^{23}$ ,  $COR^{23}$ ,  $COR^{22}$ ,  $CONR^{24}R^{25}$ ,  $SO_2R^{22}$ ,  $SO_2R^{22}$ ,  $SO_2NR^{24}R^{25}$ ,  $NR^{26}SO_2R^{22}$ ,  $B(OH)_2$ ,  $SR^{21}$ , halogen, nitro or cyano, (2) oxo, (3)  $OR^{21}$ , (4)  $OCOR^{22}$ , (5)  $OCOOR^{23}$ , (6)  $NR^{24}R^{25}$ , (7)  $NR^{26}COR^{22}$ , (8)  $NR^{26}CONR^{24}R^{25}$ , (9)  $NR^{26}COOR^{23}$ , (10)  $COOR^{23}$ , (11)  $COR^{22}$ , (12)  $CONR^{24}R^{25}$ , (13)  $SO_2R^{22}$ , (14)  $SOR^{22}$ , (15)  $SO_2NR^{24}R^{25}$ , (16)  $NR^{26}SO_2R^{22}$ , (17)  $B(OH)_2$ , (18)  $SR^{21}$ , (19) halogen, (20) nitro, (21) cyano or (22) ring E;

R<sup>21</sup> represents (i) hydrogen, (ii) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl which may be substituted with COR<sup>22</sup>, NR<sup>24</sup>R<sup>25</sup> or ring E, or (iii) ring E;

R<sup>22</sup>, R<sup>23</sup>, R<sup>24</sup>, R<sup>25</sup> and R<sup>26</sup> each independently represents (i) hydrogen, (ii) C1-15 alkyl, C2-15 alkenyl or C2-15 alkynyl which may be substituted with ring E, or (iii) ring E;

ring E represents a C3-15 monocyclic, bicyclic or tricyclic carbocyclic group, or a 5- to 15-membered monocyclic, bicyclic or tricyclic heterocyclic group which contains 1 to 4 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom, and

ring E may be substituted with 1 to 5 of (i) C1-15 alkyl which may be substituted with phenyl, (ii) halogen, (iii) phenyl, (iv) C1-15 alkoxy, (v) hydroxyl, (vi) amino, (vii) mono(C1-8 alkyl)amino, or (viii) di(C1-8 alkyl)amino;

ring A<sup>A</sup> may be substituted with 1-5 of R<sup>a</sup>; ring B<sup>A</sup> may be substituted with 1-5 of R<sup>b</sup>;

R<sup>a</sup> and R<sup>b</sup> each independently represents a group which has the same meaning as the group represented by R<sup>3</sup>; and

wherein the following compounds (1) to (6) are excluded:

- (1) N-[4-(4-morpholinyl)-2-quinazolinyl]-1,2-ethanediamine dihydrochloride,
- (2) N,N-dimethyl-N'-[2-(4-phenyl-1-piperidinyl)-4-pyrimidinyl]-1,2-ethylenediamine,
- (3) N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-[2-(1-piperidinyl)-4-pyrimidinyl]-1,3-propanediamine,
- (4) N-[(3,4-dihydro-2H-1-benzopyrane-2-yl)methyl]-N'-[2-(1-piperidinyl)-4-pyrimidinyl]-1,3-propanediamine oxalate,
- (5) N,N-diethyl-N'-[2-(1-pyrrolidinyl)-4-quinazolinyl-1,2-ethanediamine, and
- (6) N,N-diethyl-N'-[2-(1-pyrrolidinyl)-4-quinazolinyl-1,2-ethanediamine dihydrochloride,

a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof.

8. A compound represented by formula (I-B):

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&$$

wherein ring A<sup>B</sup> represents a 7- to 15-membered monocyclic, bicyclic or tricyclic heterocyclic group which is saturated or contains one double bond and which contains at least one nitrogen atom and may further contain 1 to 3 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom;

ring B<sup>B</sup> represents:

wherein ring Z represents a C5-10 monocyclic or bicyclic carbocyclic group, or a 5- to 10-membered monocyclic or bicyclic heterocyclic group which may contain 1 or 2 nitrogen atoms, one oxygen atom and/or one sulfur atom; the upward arrow represents a binding position to ring A<sup>B</sup>; and the right-downward arrow represents a binding position to the nitrogen atom bound to L;

ring  $A^B$  may be substituted with 1 to 5 of  $R^a$ ; ring  $B^B$  may be substituted with 1 to 5 of  $R^b$ ; and  $R^a$ ,  $R^b$  and other symbols have the same meanings as those described in claim 7, and

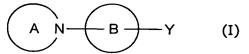
wherein the following compounds (1) to (7) are excluded:

- (1) N-[4-(hexahydro-1H-azepin-1-yl)thieno[3,2-d]pyrimidin-2-yl]-1,4-butandiamine dihydrochloride,
- (2) 7-[4-[4,6-bis(hexahydro-1H-azepin-1-yl)-1,3,5-triazin-2-yl]amino-2H-1,2,3-triazol-2-yl]-3-phenyl-2H-1-benzopyran-2-one,
- (3) 4-ethoxy-6-(hexahydro-1H-azepin-1-yl)-N-[3-(4-morpholinyl)propyl]-1,3,5-triazin-2-amine,
- (4) 4-(hexahydro-1H-azepin-1-yl)-6-methyl-N-[3-(4-morpholinyl)propyl]-1,3,5-triazin-2-amine,

- (5) 4-chloro-6-(hexahydro-1H)-azepin-1-yl)-N-[2-(4-morpholinyl)ethyl]-1,3,5-triazin-2-amine,
- (6) 4-(hexahydro-1H-azepin-1-yl)-6-methoxy-N-[3-(4-morpholinyl)propyl-1,3,5-triazin-2-amine, and
- (7) N-[4-(hexahydro-1H-azepin-1-yl)thieno[3,2-d]pyrimidin-2-yl-1,4-butanediamine, or

a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof.

- 9. The compound according to any one of claims 1, 7 and 8, which is
- (1) N-(4-azepan-1-ylpyrimidin-2-yl)ethane-1,2-diamine,
- (2) N<sup>1</sup>-(4-azepan-1-ylpyrimidin-2-yl)-N<sup>2</sup>,N<sup>2</sup>-dimethylethane-1,2-diamine,
- (3) 4-azepan-1-yl-N-((3S)-1-cyclohexylpyrrolidin-3-yl)pyrimidin-2-amine,
- (4) 4-azepan-1-yl-N-((3S)-1-benzylpyrrolidin-3-yl)pyrimidin-2-amine,
- (5) 4-azepan-1-yl-N-((3S)-1-(2-ethylbutyl)piperidin-3-yl)pyrimidin-2-amine,
- (6) 4-azepan-1-yl-N-[(3S)-1-cyclohexylpiperidin-3-yl]pyrimidin-2-amine,
- (7) 4-azepan-1-yl-N-[(3S)-1-tetrahydro-2H-pyran-4-ylpiperidin-3-yl]pyrimidin-2-amine,
- (8) 4-(3S)-3-[(4-azepan-1-ylpyrimidin-2-yk)amino]piperidin-1-ylcyclohexanol, or
- (9) (3S)-N-(4-azepan-1-ylpyrimidin-2-yl)-1'-(cyclohexylcarbonyl)-1,4'-bipiperidin-3-amine.
- 10. A pharmaceutical composition, which comprises a compound represented by formula (I):



wherein all symbols have the same meanings as those described in claim 1, a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof.

- 11. The pharmaceutical composition according to claim 10, which is a CXCR4 regulating agent.
- 12. The pharmaceutical composition according to claim 11, wherein the CXCR4 regulating agent is a CXCR4 antagonist.
- 13. The pharmaceutical composition according to claim 12, which is a preventive and/or therapeutic agent for human immunodeficiency virus infection.

- 14. The pharmaceutical composition according to claim 13, which is a preventive and/or therapeutic agent for acquired immunodeficiency syndrome.
- 15. The pharmaceutical composition according to claim 10, which is an agent for regeneration medicine.
- 16. The pharmaceutical composition according to claim 15, wherein the agent for regeneration medicine is an agent for transplantation medicine.
- 17. A CXCR4 regulating agent, which comprises a compound represented by formula (II):

wherein T represents

wherein R<sup>101</sup> and R<sup>102</sup> each independently represents hydrogen or a hydrocarbon group which may have a substituent(s); ring A has the same meaning as that described in claim 1; and other symbols have the same meanings as those described in claim 1,

a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof, as an active ingredient.

- 18. The agent according to claim 17, wherein the CXCR4 regulating agent is a CXCR4 antagonist.
- 19. A CXCR4 regulating agent, which comprises a compound represented by formula (I-3):

wherein ring A<sup>2</sup> represents a 4- to 15-membered monocyclic, bicyclic or tricyclic heterocyclic group which contains at least one nitrogen atom and may further contain 1 to 3 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom; ring B<sup>2</sup> represents a 5- to 15-membered monocyclic, bicyclic or tricyclic heterocyclic group which

contains at least one nitrogen atom and may further contain 1 to 3 nitrogen atoms, 1 or 2 oxygen atoms and/or one sulfur atom; ring  $A^2$  may be substituted with 1 to 5 of  $R^a$ ; ring  $B^2$  may be substituted with 1 to 5 of  $R^b$ ; and  $R^a$ ,  $R^b$  and other symbols have the same meanings as those described in claim 7,

a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof, as an active ingredient.

- 20. The CXCR4 regulating agent according to claim 19, which is a CXCR4 antagonist.
- 21. A CXCR4 regulating agent, which comprises the compound represented by formula (I-A) according to claim 7, a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof, as an active ingredient.
- 22. The CXCR4 regulating agent according to claim 21, which is a CXCR4 antagonist.
- 23. A CXCR4 regulating agent, which comprises the compound represented by formula (I-B) according to claim 8, a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof, as an active ingredient.
- 24. The CXCR4 regulating agent according to claim 23, which is a CXCR4 antagonist.
- 25. The CXCR4 regulating agent according to claim 17 or 19, which is a preventive and/or therapeutic agent for inflammatory/immune diseases, allergic diseases, infectious diseases, HIV infection or diseases accompanied therewith, psychoneurotic diseases, cerebral diseases, cardiovascular diseases, metabolic diseases and cancerous diseases.
- 26. The CXCR4 regulating agent according to claim 25, which is a preventive and/or therapeutic agent for HIV infection or diseases accompanied therewith.
- 27. The CXCR4 regulating agent according to claim 17 or 19, which is useful for regeneration medicine.

- 28. A medicament which comprises the compound according to any one of claims 1, 7, 8 and 17, a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof, in combination with one or at least two of a reverse transferase inhibitor, a protease inhibitor, a CCR2 antagonist, a CCR3 antagonist, a CCR4 antagonist, a CCR5 antagonist, a fusion inhibitor, an antibody against a surface antigen of HIV-1, and a vaccine of HIV-1.
- 29. The medicament according to claim 28, wherein the reverse transferase inhibitor is one or at least two selected from zidovudine, didanosine, zalcitabine, stavudine, lamivudine, abacavir, adefovir, dipivoxil, emtricitabine, tenofovir, nevirapine, nevirapine, efavirenz and capravirine.
- 30. The medicament according to claim 28, wherein the protease inhibitor is one or at least two selected from indinavir, ritonavir, nelfinavir, saquinavir, amprenavir, lopinavir and lopinavir.
- 31. A method for antagonizing CXCR4 in a mammal, which comprises administering to a mammal an effective amount of a compound represented by formula (II):

wherein all symbols have the same meanings as those described in claim 1 or 17,

a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof,

32. Use of a compound represented by formula (II):

wherein all symbols have the same meanings as described in claim 1 or 17, a salt thereof, an N-oxide thereof, a solvate thereof, or a prodrug thereof for the manufacture of a CXCR4 antagonist.